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NOTE

NUMIT-ONE AMENDMENT #2
(FOR THE SDS 920)

AFRRI TN68-3

ARMED FORCES RADIOBIOLOGY RESEARCH INSTITUTE
Defense Atomic Support Agency
Bethesda, Maryland

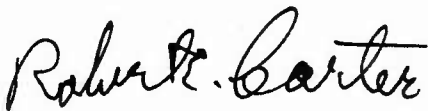
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NUMIT-ONE AMENDMENT #2

(FOR THE SDS 920)

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TABLE OF CONTENTS

	Page
Foreword (Nontechnical summary)	iii
Abstract	iv
I. Introduction	1
II. Accuracy	1
III. Input Limitations	2
IV. Input and Output Formats	3
V. Operation	4
References	5
Appendix A	7
Appendix B	9
Figure 1	10

FOREWORD
(Nontechnical summary)

This report describes a numerical integration program much like the amended form of NUMIT-ONE but written for the SDS 920, a faster and larger computer. While the flow chart is identical to the amended version of NUMIT-ONE, the coding has taken advantage of the more flexible SDS FORTRAN II and the input and output devices have been changed to paper tape since this is standard equipment for SDS 900 series computers and a card read-punch is not available for our SDS 920.

ABSTRACT

An amendment to NUMIT-ONE is presented. The program utilizes Simpson's Rule to perform integration over any closed intervals on the SDS 920.

I. INTRODUCTION

NUMIT-ONE, originally coded for the IBM 1620, has now been recoded for the SDS 920. The code follows the flow chart given in the NUMIT-ONE amendment.^{1, 2} The code itself approximately duplicates the IBM 1620 code; the only changes being those to take advantage of SDS FORTRAN II and input/output instructions. Familiarity with both of the previous publications is assumed.

Equipment needed:

FORTRAN II Processor

SDS 920 with minimum 4 K memory

While it has not been attempted, this program could probably be compiled and run on a smaller SDS computer of the 900 series.

II. ACCURACY

Floating point quantities in the 920 are held to approximately 12 digits unlike the IBM 1620 where variable precision parameters are possible. Generally, one can obtain six significant figures, the maximum output precision now called for.

Proper analysis prior to attempting to integrate, e.g., plotting data to visually select subintervals of integration, will have the double benefit of improving accuracy and reducing machine time. The test case in Appendix B illustrates this. On the first run the total interval was broken into three parts, with each subinterval carefully chosen so that unnecessary extremes would not be reached in any interval and the results for the parts were summed after the three passes. The result is an answer accurate to approximately six significant figures in a few minutes of machine time.

One can integrate over the entire interval in cases when time for analysis is short; that is, when plotting and other manual analysis is not possible. However, the second run of the test case in Appendix B using the entire interval method took over twice as much machine time and the result was slightly less accurate than the previous run after 14 iterations. Analysis is important when time permits.

A word of caution about the limits of integration: a situation in which the program will break down occurs when integrating over an interval where the integrand takes on both positive and negative values and produces an integral close to zero. In such cases, significant figures will be lost during integrating and DELTA J will exhibit a wild behavior instead of converging rapidly as it should. In a case like this, it is best to split the integrand into at least two parts, each containing a nonzero part of the total integral.

III. INPUT LIMITATIONS

Input limitations are the same as for the amended NUMIT-ONE for the IBM 1620 with one exception. J_{\max} for this version must not be more than 24 due to limits on the size of fixed point quantities in SDS FORTRAN II. Generally this allows for more iterations than one would be willing to use.

The integrand, $f(x)$, is provided by a subprogram of the FUNCTION type called FUN (X,N). X, computed in the main program, is the value of X when the function is called on; N* is the 'pass number'. FUN must appear on the left of an arithmetic statement equivalent to the integrand in the subprogram before returning to the main program.

* The integral is evaluated over several separate X regions as a sum of several independent integrals over disjoint regions; the integer variable describing the separate integrals is N.

IV. INPUT AND OUTPUT FORMATS

Input Format

Input is by paper tape. The following quantities are specified in the input (floating point quantities are in lower case, fixed point quantities in upper case).

a = lower limit of interval

b = upper limit of interval

J_{max} = maximum number of iterations desired

Δ = convergence criterion (floating point)

Line 1

Alpha Identification. Reproduced in the output and does not affect processing. Up to 80 characters permitted.

Line 2

Integrand Specification. Contains alphanumeric information to identify integrand in output. This does not affect processing. Up to 48 characters permitted.

Line 3

		<u>Format</u>
Columns 1-11	a	E 11.6
Columns 12-22	b	E 11.6
Columns 23-25	J _{max}	I 3
Columns 26-33	Δ	F 8.6
Columns 34-35	Switch	F 2.0

Following line 3 may be any number of additional lines with new values of a, b, J_{max}, and Δ punched according to the same formats. If more lines follow, switch must be punched. If no lines follow, switch should not be punched. In the last line, switch must not be punched.

Errors in Input

All the error checks listed in AFRRI SR65-1 are made, with one change. J_{\max} is permitted to be as high as 24 instead of 11 before an error message will be punched and the computer halts.

Output Format

Output is identical to the amended form of NUMIT-ONE for the IBM 1620, the only change being that output is on paper tape rather than cards.

Two sample listings are in Appendix B.

V. OPERATION

Operation is routine. The standard FORTRAN II compiler is used and no switches are utilized.

REFERENCES

1. Rockwell, R. W. and Garrett, C. W. NUMIT-ONE; a numerical integration program in one-dimension for the IBM 1620 Computer. Bethesda, Maryland, Armed Forces Radiobiology Research Institute Scientific Report SR65-1, 1965.
2. Rockwell, R. W. NUMIT-ONE Amendment #1. Bethesda, Maryland, Armed Forces Radiobiology Research Institute Technical Note TN68-1, 1968 (in press).

APPENDIX A

Source Program

```

= 1 C NUMIT ONE - ROCKWELL - NOV, 1965
= 2 DIMENSION F[0/2],P[0/2],Q[0/2],U[6]
= 3 P[0]=1.
= 4 P[1]=4.
= 5 P[2]=1.
= 6 Q[0]=1.
= 7 Q[1]=2.
= 8 Q[2]=1.
= 9 N=0
= 10 TOTAL = 0.
= 11 ACCEPT TAPE 100
= 12 PUNCH TAPE 100
= 13 PUNCH TAPE 101
= 14 ACCEPT TAPE 107, [U[i],i=1,6]
= 15 PUNCH TAPE 108, [U[i],i=1,6]
= 16 1 ACCEPT TAPE 102,A,B,JMAX,DELTA1,SW1
= 17 IF[IF[A,B]]3,2,3
= 18 2 PUNCH TAPE 103
= 19 STOP
= 20 3 IF[DELTA1]5,4,5
= 21 4 PUNCH TAPE 104
= 22 STOP
= 23 5 IF[JMAX-24]7,7,6
= 24 6 PUNCH TAPE 105
= 25 STOP
= 26 7 IF[JMAX-2]6,8,8
= 27 8 SUM1=0.
= 28 SUM=0.
= 29 N=N+1
= 30 J=1
= 31 K2=2
= 32 PUNCH TAPE 106,B,JMAX,A,DELTA1
= 33 9 DELX=[B-A]/[2,**J]
= 34 IF[J-1]10,10,14
= 35 10 DO 11 I=0,2
= 36 X=A+I*DELX
= 37 F[I]=FUN[X,N]
= 38 SUM1=SUM1+Q[I]*F[I]
= 39 11 SUM =SUM + P[I]*F[I]
= 40 AN1=DELX*SUM/3.
= 41 J=J+1
= 42 GO TO 9
= 43 14 SUM=0.
= 44 DO 15 I=1,K2
= 45 X=A+[2*I-1]*DELX
= 46 15 SUM = SUM+FUN[X,N]
= 47 AN2 = DELX*[4.*SUM+SUM1]/3.
= 48 DELTA = ABSF[(AN1-AN2)/AN2*100.]
= 49 IF[DELTA-DELTA1]19,19,16
= 50 16 IF[J-JMAX]17,19,19
= 51 17 AN1=AN2
= 52 SUM1= SUM1+2.*SUM
= 53 PUNCH TAPE 109,J,AN2,DELTA
= 54 J=J+1
= 55 K2=2*K2

```

```

= 56      GO TO 9
= 57      19 PUNCH TAPE 110,J,N,AN2,DELTA
= 58      TOTAL=TOTAL+AN2
= 59      IF(SW1)1,20,1
= 60      20 PUNCH TAPE 111,N,TOTAL
= 61      STOP
= 62      100 FORMAT(80H
= 63      1
= 64      107 FORMAT(6A8]
= 65      108 FORMAT(15X,$F[X] = $,6A8]
= 66      101 FORMAT(/15X,$NUMIT ONE [ONE-DIM. INTEGRATION, SIMPSONS RULE]$]
= 67      102 FORMAT(2E11.6,13,F8.6,F2.0]
= 68      103 FORMAT(10X,$CHECK INPUT - A=B$]
= 69      104 FORMAT(10X,$CHECK INPUT - DELTA = 0$]
= 70      105 FORMAT(10X,$CHECK INPUT - JMAX OUTSIDE RANGE$ ]
= 71      106 FORMAT(/35X,$INPUT DATA$/21X,$B = $1PE12.5,9X,$J[ MAX] = $13/
= 72      121X,$A = $1PE12.5,9X,$DELTA1 = $1PE10.4//16X,$ITEPATION$,11X,
= 73      2$INTEGRAL$,13X,$DELTA$]
= 74      109 FORMAT(18X,13,12X,1PE12.5,8X,0PF10.4]
= 75      110 FORMAT(18X,13,$[PASS$,12,$1$,4X,1PE12.5,8X,0PF10.4///]
= 76      111 FORMAT(32X$NO. PASSES = $13/29X$TOTAL INTEGRAL= $1PE12.5/
= 77      139X$END$]
= 78      END

```

PROGRAM ALLOCATION

00007 F	00015 P	00023 Q	00031 U
00045 N	00046 I	00047 JMAX	00050 J
00051 K2	00052 TOTAL	00054 A	00056 B
00060 DELTA1	00062 SW1	00064 SUM1	00066 SUM
00070 DELX	00072 X	00074 AN1	00076 AN2
00100 DELTA			

SUBPROGRAMS REQUIRED

IF FUN ABSF

THE END

APPENDIX B

Test Case

Running time is still highly variable and depends strongly on the integrand. However, time is much shorter than on the IBM 1620. No case is known which is not at least 15 times as fast on the SDS 920 as on the other computer, the ratio being highest when the number of iterations is large. The formula given in the previous reports,

$$t = K \cdot 2^{J_{act}}$$

where K is a constant dependent on the integrand, still appears to be valid when the number of iterations is large enough so the time spent computing is large compared to the time spent punching tape.

The function illustrated here,

$$f(x) = x^7 \frac{\sqrt{1-x^2}}{(2-x)^{13/2}}$$

has been the most difficult tested thus far. It converges slower and the value of K (7.47×10^{-4} sec) is larger than any heretofore reported. Figure 1 illustrates the function over the intervals of -1 to 1. Running time for RUN 1 was 5.5 minutes; RUN 2 took 12.25 minutes.

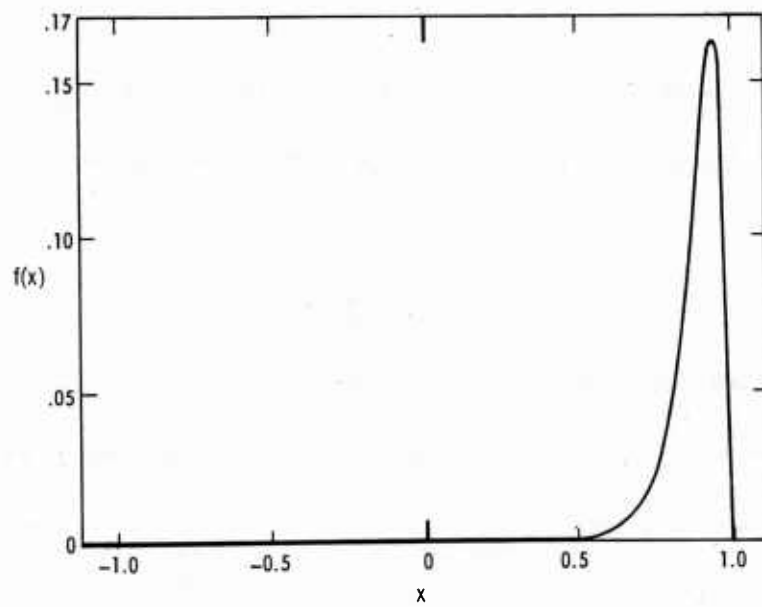


Figure 1

```

C      SOURCE STATEMENTS OF SUBROUTINE
C
      FUNCTION FUN(X,N)
      FUN=X**7*SQRTE(1.-X*X)/(2.-X)**6.5
      RETURN
      END

```

INPUT DATA

RUN 1

```

      X**7*SQRTE(1-X*X)/(2-X)**13/2      TEST FUNCTION
-1000000+01,+500000+00,12,.010000,1,
+500000+00,+800000+00,12,.001000,1,
+800000+00,+100000+01,12,.000100,

```

RUN 2

```

      X**7*SQRTE(1-X*X)/(2-X)**13/2      TEST FUNCTION
-1000000+01,+100000+01,14,.000500,

```


OUTPUT DATA

RUN 1

TEST FUNCTION

NUMIT ONE [ONE-DIM. INTEGRATION, SIMPSONS RULE]
 $F[X] = X^{**7} * \text{SQRT}(1 - X * X) / (2 - X)^{**13/2}$

INPUT DATA

B = 5.000000E-01 J[MAX] = 12
A = -1.000000E 00 DELTA1 = 9.9999E-03

ITERATION	INTEGRAL	DELTA
2	3.31206E-05	265.1566
3	-1.74285E-05	290.0372
4	-3.03975E-05	42.6647
5	-3.29935E-05	7.8681
6	-3.36745E-05	2.0223
7	-3.38945E-05	0.6491
8	-3.39703E-05	0.2231
9	-3.39968E-05	0.0781
10	-3.40062E-05	0.0275
11[PASS 1]	-3.40095E-05	0.0097

INPUT DATA

B = 7.99999E-01 J[MAX] = 12
A = 5.00000E-01 DELTA1 = 9.9999E-04

ITERATION	INTEGRAL	DELTA
2	2.90366E-03	3.5586
3	2.89730E-03	0.2193
4	2.89694E-03	0.0126
5[PASS 2]	2.89692E-03	0.0008

INPUT DATA

B = 1.00000E 00 J[MAX] = 12
A = 7.99999E-01 DELTA1 = 9.9999E-05

ITERATION	INTEGRAL	DELTA
2	1.95064E-02	16.7288
3	2.05071E-02	4.8794
4	2.08279E-02	1.5404
5	2.09361E-02	0.5167
6	2.09735E-02	0.1784
7	2.09866E-02	0.0624
8	2.09912E-02	0.0219
9	2.09928E-02	0.0077
10	2.09934E-02	0.0027
11	2.09936E-02	0.0010
12[PASS 3]	2.09936E-02	0.0003

NO. PASSES = 3
TOTAL INTEGRAL= 2.38566E-02
END

RUN 2

TEST FUNCTION

NUMIT ONE [ONE-DIM, INTEGRATION, SIMPSONS RULE]
 $F[X] = X^{**7} * \text{SQRT}(1 - X * X) / (2 - X)^{**13/2}$

INPUT DATA

B = 1.00000E 00 J[MAX] = 14
A = -1.00000E 00 DELTA1 = 4.9999E-04

ITERATION	INTEGRAL	DELTA
2	3.11637E-04	100.0000
3	6.93780E-03	95.5081
4	1.70652E-02	59.3454
5	2.17058E-02	21.3795
6	2.31639E-02	6.2948
7	2.36230E-02	1.9433
8	2.37758E-02	0.6426
9	2.38283E-02	0.2204
10	2.38466E-02	0.0769
11	2.38531E-02	0.0270
12	2.38554E-02	0.0095
13	2.38562E-02	0.0034
14[PASS 1]	2.38564E-02	0.0012

NO. PASSES = 1
TOTAL INTEGRAL= 2.38564E-02
END

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